# Dynamical description of the buildup process in resonant tunneling: evidence of exponential and non-exponential contributions

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The buildup process of the probability density inside the quantum well of a double-barrier resonant structure is studied by considering the analytic solution of the time dependent Schrödinger equation with the initial condition of a cutoff plane wave. For one level systems at resonance condition we show that the buildup of the probability density obeys a simple charging up law, $|\Psi(\tau)/\phi| = 1-e^{-\tau/\tau_0}$, where $\phi$ is the stationary wave function and the transient time constant $\tau_0$ is exactly two lifetimes. We illustrate that the above formula holds both for symmetrical and asymmetrical potential profiles with typical parameters, and even for incidence at different resonance energies. Theoretical evidence of a crossover to non-exponential buildup is also discussed.

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Since the pioneering work of Esaki and Tsu [1], the tunneling in one-dimensional semiconductor heterostructures has been the subject of intense investigations [2,3,4,5]. Resonant tunneling in double barrier (DB) systems has received special attention both by its technological applications and by the motivation to clarify the new interesting transport phenomena. Among the fundamental problems that have appeared on the scene, the charge buildup in the quantum well region is considered as one of the most important processes since it governs the ultimate speed of resonant tunneling devices [3,4]. The need of a direct and comprehensive dynamical study of this phenomenon has been widely recognized [4,5,6]. However, up to now we are lacking of an exact description of the buildup process itself.

In this paper we provide an exact description of the buildup process at resonance condition, within the framework of the shutter model. This is based on a full quantum dynamical approach, recently developed by García-Calderón and Rubio [7], that deals with the solution of the time dependent Schrödinger equation for an arbitrary potential $V(x)$ $(0<x<L)$, with an initial condition of a cutoff plane wave confined in the half-space $x<0$ to the left of an absorbing shutter [9] at $x=0$. The sudden opening of the shutter at $t=0$ allows the wave function to interact with the potential. As a consequence, they found that the transient solution for the internal region may be written as the stationary solution modulated by a time varying Moshinsky function plus an infinite sum of transient resonance terms associated with the $S-$matrix poles of the problem.

For the case of a reflecting shutter

$$\Psi(x,k;t=0) = \begin{cases} e^{ikx}-e^{-ikx} & -\infty < x \leq 0 \\ 0 & x>0, \end{cases} \tag{1}$$

one can proceed along the lines similar to that discussed in Ref. [7] and obtain the solution for the internal region,

$$\Psi(x,k;t) = \phi(x,k)M(0,k;t) - \phi^*(x,k)M(0,-k;t) -i\sum_{n=-\infty}^{\infty} T_n M(0,k_n;t), \tag{2}$$

where $\phi(x,k)$ is the stationary wave function and the factors $T_n = 2ku_n(0)u_n(x)/(k^2-k_n^2)$ are given in terms of the resonant eigenfunctions $u_n(x)$. The index $n$ runs over the complex poles $k_n$ distributed in the third and fourth quadrants in the complex $k$-plane. The Moshinsky functions [7], as it is well known, are defined in terms of the complex error function $w(z)$ [10]: $M(y_q) \equiv M(0,q;t) = w(iy_q)/2$, where the argument $y_q$ is given by

$$y_q = -e^{-i\pi/4}\left(\frac{m}{2\hbar}\right)^{1/2}\left[\frac{\hbar q}{m}t^{1/2}\right], \tag{3}$$

and $q$ stands either for $\pm k$ or $k_{\pm n}$.

The time evolution of wavefunction $\Psi(x,k;t)$ in the internal region may be described by the expression given by Eq. (2), which involves the contribution of the full resonant spectrum of the system. For structures with typical parameters, and incidence energies $E=\hbar^2k^2/2m$ near a resonance energy $\varepsilon_n$, García-Calderón and Rubio [7] showed that the single resonance approximation for the wavefunction $\Psi(x,k;t)$ is valid from a few tenths of the corresponding lifetime onwards. This is the case for the present study, since we are not considering the regime of very short times ($t \ll \tau_n = \hbar/\Gamma_n$), which may require the contribution of far away resonances. The single resonance approximation to Eq. (2) is

$$\Psi(x,k;t) = \phi(x,k)M(0,k;t) - \phi^*(x,k)M(0,-k;t) -iT_nM(0,k_n;t) - iT_{-n}M(0,-k_n^*;t), \tag{4}$$

where we have used the fact that the poles in the third quadrant $k_{-n}$ are related to those of the fourth, $k_n$, by $k_{-n} = -k_n^*$. This is the one-level expression of the time dependent wave function for the description of the dynamics in the internal region.

In order to exemplify the building up of the probability density in the quantum well for incidence at different resonance energies and for different potential profiles, let us consider the following two numerical examples. The first case corresponds to the symmetrical DB structure with parameters: barrier heights $V_0 = 0.5$ $eV$, barrier widths $b_0 = 30$ Å and well width $\omega_0 = 100$ Å. The resonance parameters for the first three resonant states are: $\varepsilon_1 = 37.8$ $meV$, $\Gamma_1 = 0.12$ $meV$; $\varepsilon_2 = 149.2$ $meV$, $\Gamma_2 = 1.40$ $meV$; $\varepsilon_3 = 325.7$ $meV$, $\Gamma_3 = 8.60$ $meV$. We show in Fig. 1 the time evolution of the probability density calculated by Eq. (4) for incidence at resonance, $E = \varepsilon_n$ and fixed position $x$ (we have considered values of $x$ near the maxima of $|\phi(x,k)|^2$ as the most natural choice) for the cases: $n = 1$, $x = 80$ Å (solid line); $n = 2$, $x = 48$ Å (dashed line); and $n = 3$, $x = 80$ Å (dotted line). The second example consists of an asymmetrical DB structure with parameters: barrier heights $V_1 = V_2 = 0.3$ $eV$, barrier widths $b_1 = 30$ Å and $b_2 = 100$ Å, and well width $\omega_0 = 50$ Å. The resonance parameters for the first resonant state are $\varepsilon_1 = 89.1$ $meV$ and $\Gamma_1 = 2.4$ $meV$. The time evolution of $|\Psi(x,k;t)|^2$ for incidence at $E = \varepsilon_1$ and $x = 55$ Å is also depicted in Fig. 1 (dashed-dotted line). For all cases, the probability density $|\Psi(x,k;t)|^2$ grows up monotonically towards its asymptotic value. We can see that both the level off and the rate of increase of the curves are quite different. However, a common feature, not evident in Fig. 1, can be appreciated if we replot the normalized probability density $|\Psi(x,k;\tau)/\phi(x,k)|^2$ as a function of the new variable $\tau$, which is now the time given in lifetime units ($t$ replaced by $\tau\hbar/\Gamma_n$ for each curve). As a result, all four curves become indistinguishable among them as depicted in Fig. 2. We can see that the full establishment of the stationary situation is preceded by a transient in which the probability density is built up inside the quantum well with a unique characteristic curve. Thus, there must also exist a characteristic transient time constant $\tau_0$ that governs the buildup process, with the same value (in lifetimes) for all cases. The observed regularity and the fact that it holds for both symmetrical and asymmetrical cases and at different resonances, is a manifestation that the buildup process in one-level systems is governed by a simple law. In what follows we shall be concerned to find the analytic expression of the actual buildup law and the exact value of the characteristic transient time $\tau_0$.

For sharp ($R_n \equiv \varepsilon_n/\Gamma_n \gg 1$) and isolated resonances we know that the stationary wavefunction $\phi(x,k)$ can be written as the one-term expression [11] $\phi(x,k) = 2iku_n(0)\,u_n(x)/(k^2 - k_n^2)$, thus the factors $iT_n$ and $iT_{-n}$ appearing in Eq. (4) can be identified as $\phi(x,k)$ and $-\phi^*(x,k)$ respectively. By expressing formula (3) in lifetime units, it can be seen that $y_q$ depends only on the ratio $R_n = \varepsilon_n/\Gamma_n$, and not on the particular values of the resonance parameters $\varepsilon_n$ and $\Gamma_n$. For $q = \pm k_n$ and $q = \pm k_n^*$, $y_q$ reads: $y_{\pm k_n} = \mp e^{-i\pi/4}\left[(R_n - i/2)\,\tau\right]^{1/2}$, and $y_{\pm k_n^*} = \mp e^{-i\pi/4}\left[(R_n + i/2)\,\tau\right]^{1/2}$, respectively. For the cases $q = \pm k$ we have $y_{\pm k} = \mp e^{-i\pi/4}\left[R_n\tau\right]^{1/2}$ (since $E = \varepsilon_n$). From the above considerations and the well known symmetry relation [7], $M(y_q) = e^{y_q^2} - M(-y_q)$, applied to the Moshinsky functions $M(y_k)$ and $M(y_{k_n})$, we obtain a convenient representation for the probability density,

$$|\Psi(x,k;\tau)|^2 = |\phi(x,k)|^2\,(1 - e^{-\tau/2})^2 + \Delta(\tau), \tag{5}$$

where $\Delta(\tau)$ stands for the remaining terms, which involve the square modulus of the Moshinsky functions and several interference terms. It is not difficult to convince oneself that, for very large times, expression (5) possesses the correct asymptotic behavior, *i. e.* as $\tau \to \infty$, $|\Psi(x,k;\tau)|^2$ goes into the stationary probability density $|\phi(x,k)|^2$. This follows directly from the presence of the decreasing exponential $e^{-\tau/2}$, and from the fact that each of the Moshinsky functions involved in $\Delta(\tau)$ can be represented by a series expansion consisting of inverse powers of $\tau$. In Ref. [7] it was shown that $M(y_q)$ has the asymptotic expansion $M(y_q) = a_1/y_q + a_2/y_q^2 + a_3/y_q^3 + \cdots$ for large values of the variable $y_q$ provided that $-\pi/2 < arg(y_q) < \pi/2$. By inspection of our expressions for $y_q$, we can see that the above inequality holds for the three cases involved in $\Delta(\tau)$ ($q = -k$, $-k_n$, and $-k_n^*$), and as a consequence $\Delta(\tau) \to 0$ when $\tau \to \infty$, as expected. It is important not only that both $e^{-\tau/2}$ and $\Delta(\tau)$ go to zero, but also the fact that their rates of decrease are quite different, leading to important consequences on the nature of the buildup. In particular it reveals that there exist exponential and non-exponential contributions to the buildup mechanism, as we shall see later. In view of the series expansions considered above, $\Delta(\tau)$ also contains inverse powers of $y_q$, that is, inverse powers of the product $(R_n\tau)^{1/2}$. This means that $\Delta(\tau)$ can be vanishingly small even for $\tau$ equal to a few lifetimes, provided that $R_n \gg 1$. In fact, there exists a finite time interval in which $\Delta(\tau)/|\phi|^2$ is negligible compared to $e^{-\tau/2}$, leading to the following exponential buildup law:

$$|\Psi(\tau)/\phi| = 1 - e^{-\tau/2}. \tag{6}$$

This simple formula reproduces successfully the predicted values of expression (4). For comparison, we have included in Fig. 2 a plot of the normalized probability density calculated from (6). The corresponding curve is indistinguishable from all the other curves, showing in particular that $\Delta(\tau)$ has an exceedingly small contribution in the relevant time interval for all of our numerical examples. We see that formula (6) does not depend ex-

plicitly on the potential profile parameters nor the resonant state, this explains why all the numerical examples illustrated in Fig. 2 share the same curve, despite the fact that they correspond to different situations. Note that in the exponential regime the buildup law becomes identical to the charging up law of a capacitor in an $RC-$circuit: $Q(\tau)/Q_0 = 1 - e^{-\tau/\tau_C}$, where $Q_0$ is the asymptotic charge, and $\tau_C = RC$ is the capacitive time constant. This is relevant, because we find in the literature capacitor-like models used to describe quantum tunneling properties in DB structures, such as the charge buildup and its implications on the speed limit on resonant tunneling devices [3,12]. According to Eq. (6), the transient time constant $\tau_0$ of our "quantum capacitor" *is always two lifetimes*, and is a characteristic feature of one-level systems. On the experimental side, it is worth to mention that measured values of escape times of the order of $2\hbar/\Gamma_n$ has been reported by Sakaki *et al.* [8], arguing that, at coherence conditions, *"the buildup time and the tunneling escape time are roughly the same"* [4]. An important remark is that the condition $R_n \gg 1$ is not so restrictive since it is satisfied for most of the resonant structures with typical parameters. In fact we carried out a systematical study (not shown here) and found that for values of $R_n$ from 10 onwards this condition is satisfied.

In order to show the existence of deviations from the exponential regime, we shall examine the contributions arising from $\Delta(\tau)$. The explicit calculation of $\Delta(\tau)$ in terms of $y_{-k}$, $y_{-k_n}$, and $y_{-k_n^*}$ may result a too involved task, however, for the purpose of our discussion, it is sufficient to realize that the dominant term is proportional to an oscillatory function of $\tau$ modulated by the factor $\tau^{-1/2}$. We know that at very long times the exponential term goes to zero faster than $\tau^{-1/2}$, *i. e.* $e^{-\tau/2} \ll \tau^{-1/2}$. Therefore, there must exist a critical time $\tau_{onset}$ at which $e^{-\tau/2}$ and $\Delta(\tau)/|\phi|^2$ are comparable. Such a critical time defines a crossover from the exponential to a non-exponential regime of the buildup process. In the examples depicted in Fig. 2 the non-exponential contributions to $|\Psi(\tau)/\phi|^2$ are overwhelmed and cannot be appreciated due to the scale of the graph. However, if we plot the logarithm of the difference $\delta(\tau) = |1-|\Psi(\tau)/\phi||$ versus $\tau$, [using Eq. (4)] the transition from the exponential to the non-exponential regime is clearly appreciated, see Fig. 3. In this figure, the exponential regime can be identified by the straight line with slope $-1/2$, extending over a few lifetimes until it reaches the onset of the nonexponential buildup, $\tau_{onset}$, which depends on $R_n$.

It is interesting to note the similarity of the results depicted in Fig. 3 to the behavior of the *survival probability* found in studies of the phenomenon of quantum decay [13,14], which also exhibits this transition with an oscillatory structure at such crossover. We believe that this striking resemblance is not a simple coincidence but rather a manifestation of the existence of a more profound link between both phenomena. In fact, the survival probability may also be expressed in terms of the Moshinsky functions [13], which are, in our expressions, the key ingredients for the time evolution. These findings open up new questions about the common features in both processes, for example those about the existence of deviations from the exponential buildup also at early times, as it occurs in the decay process [15]. Such analysis requires the contribution of far away resonances to the transient solution, and is deferred to future work [16].

Summarizing: *(i)* We have accomplished the first analytic derivation of the actual buildup law in resonant tunneling structures. It was based on general properties of the solution of the Schrödinger equation, without any assumptions on the potential profile, except that it is finite and support well defined resonances. *(ii)* We have shown the existence of both exponential and non-exponential contributions to the buildup process. *(iii)* The exponential regime is characterized by a transient time constant whose value is exactly *two lifetimes*. *(iv)* We have illustrated that formula (6) describes very accurately the exponential buildup for a great variety of situations: it works very well for different potential profiles, and is valid not only for the "ground state" ($n = 1$), but also for "excited states" ($n > 1$).

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FIG. 1. This graph illustrates the building up of the probability density for the two examples discussed in the text. In the symmetrical system we show the time evolution for $|\Psi\left(x,k;t\right)|^2$ for incidence at: $\varepsilon_1 = 37.8$ $meV$ (solid line), $\varepsilon_2 = 149.2$ $meV$ (dashed line) and $\varepsilon_3 = 325.7$ $meV$ (dotted line). The fixed positions $x$ are: 80 Å, 48 Å and 80 Å, respectively. In the asymmetric case $\varepsilon_1 = 89.1$ $meV$ (dashed-dotted line) at $x = 55$ Å

FIG. 2. Evolution of $\left|\Psi\left(\tau\right)/\phi\right|^2$ as a function of $\tau$ for the same cases of Fig.1. All four curves become identical. For comparison, a plot of $\left|\Psi\left(\tau\right)/\phi\right|^2$ using Eq.(6) is also included. The resulting values are also superimposed on the other curves illustrating that they obey a simple exponential law with a unique transient time constant of two lifetimes.

FIG. 3. Exponential and non-exponential contributions to the buildup. We plot the logarithm of the difference of $\delta(\tau) = |1 - |\Psi\left(\tau\right)/\phi||$ versus $\tau$, for the states $n = 1$ and $n = 3$ of the symmetrical system considered in the text. The corresponding values of the ratios $R_n \equiv \varepsilon_n/\Gamma_n$ are show in the figure. The linear behavior corresponds to the exponential regime, and the deviations from it appear after a certain transition time $\tau_{onset}$.

Figure 1

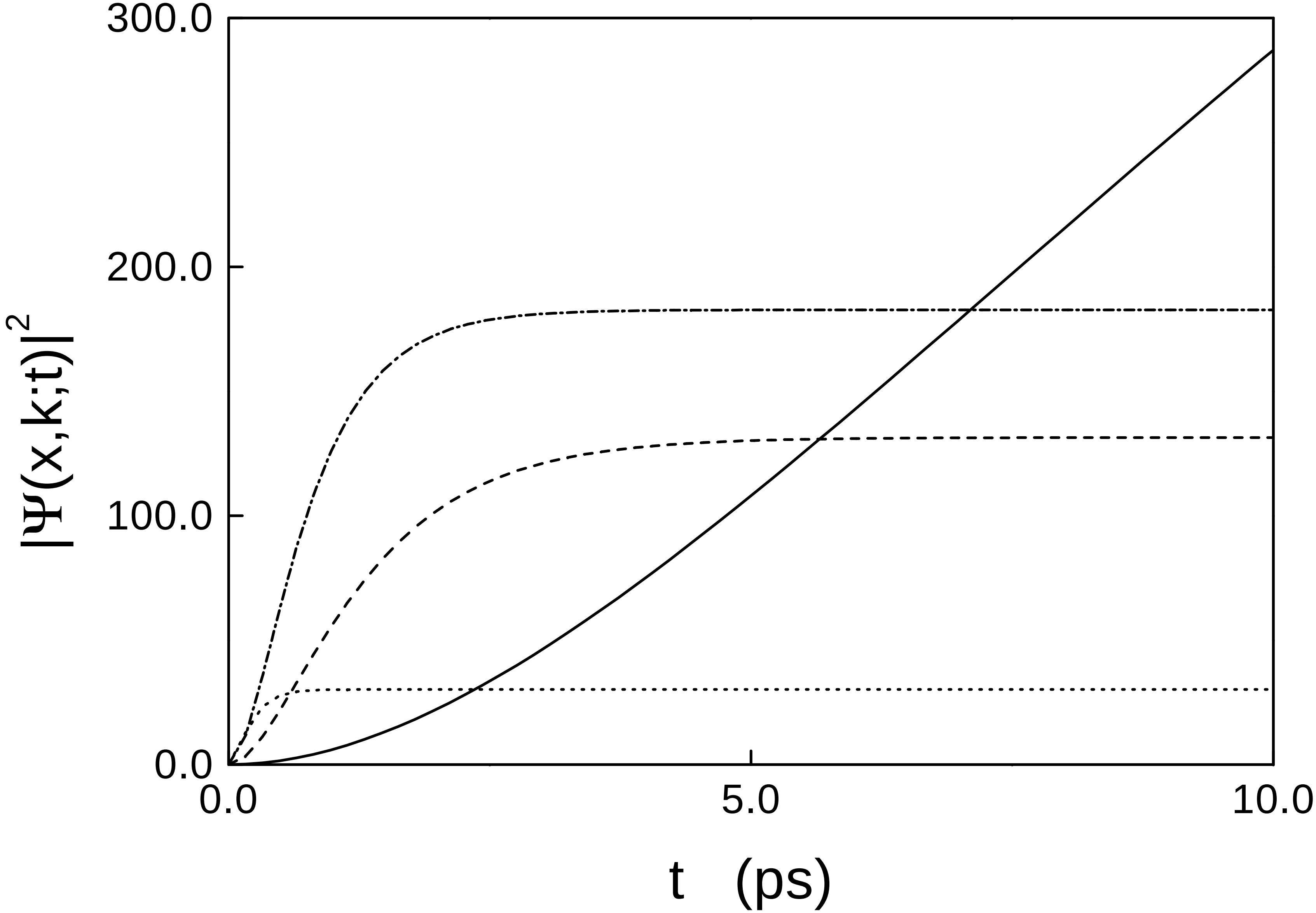
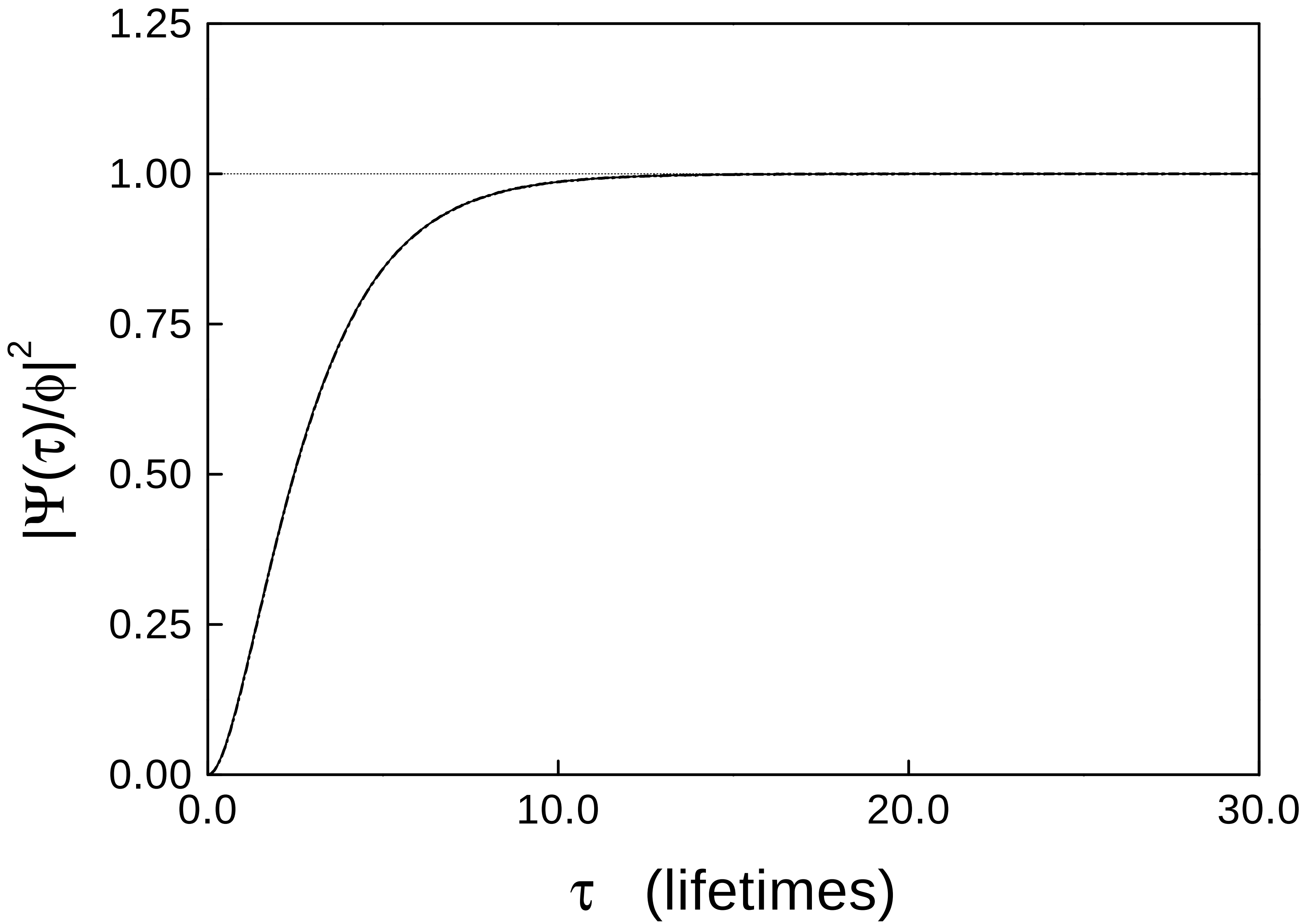
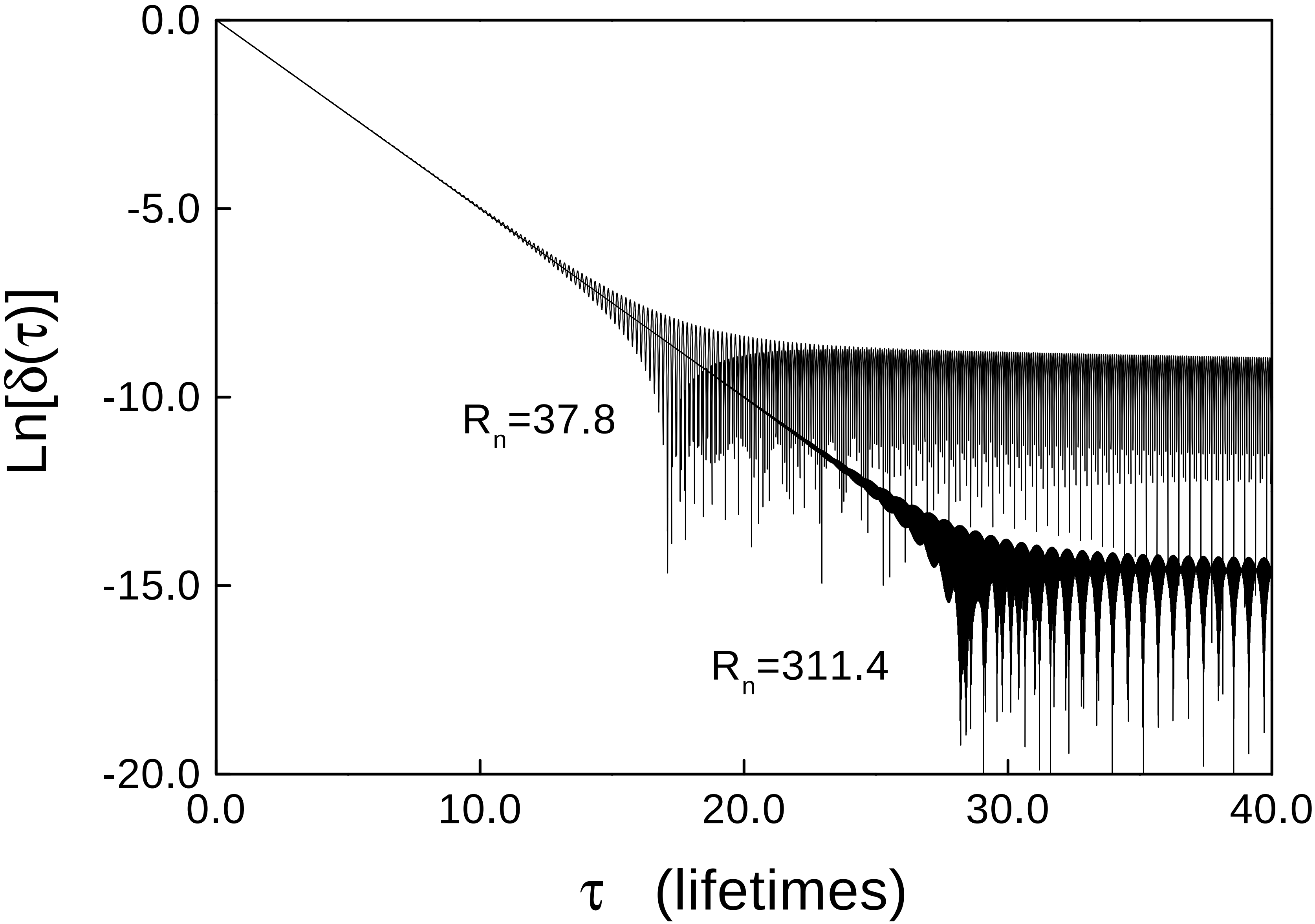


Figure 2



1.25
1.00
0.75
0.50
0.25
0.00
0.0
10.0
20.0
30.0
$|\Psi(\tau)/\phi|^2$
$\tau$ (lifetimes)

Figure 3



0.0
-5.0
-10.0
-15.0
-20.0
0.0
10.0
20.0
30.0
40.0
Ln[δ(τ)]
τ (lifetimes)
$R_n$=37.8
$R_n$=311.4